CLAIMS

1. A method for assaying a drug candidate with a biosensor having one or more sensing surface-bound biomolecules associated therewith, comprising the steps of:

measuring the binding interaction between the drug candidate and the one or more sensing surface-bound biomolecules of the biosensor to obtain at least one binding interaction parameter of the drug candidate; and

comparing the at least one binding interaction parameter against at least one mathematical expression correlated from binding interaction data associated with known drug compounds to determine an estimate of at least one pharmacokinetic parameter of the drug candidate.

2. The method of claim 1 wherein the at least one pharmacokinetic parameter is an absorption parameter, a distribution parameter, a metabolism parameter, or an excretion parameter.

3. The method of claim 1 wherein the at least one pharmacokinetic parameter is volume of distribution, total clearance, protein binding, tissue binding, metabolic clearance, renal clearance, hepatic clearance, biliary clearance, intestinal absorption, bioavailability, relative bioavailability, intrinsic clearance, mean residence time, maximum rate of metabolism, Michaelis-Menten constant, partitioning coefficients between tissues and blood or plasma, fraction excreted unchanged in urine, fraction of drug systemically converted to metabolites, elimination rate constant, half-life, or secretion clearance.

4. The method of claim 3 wherein the partitioning coefficients between tissues and blood or plasma are partitioning coefficients associated with the blood brain barrier, blood placenta barrier, blood human milk partitioning, blood adipose tissue partitioning, or blood muscle partitioning.

5. The method of claim 1 wherein an estimate of at least two pharmacokinetic parameters of the drug candidate are determined.

6. The method of claim 1 further comprising determining an estimate of a solubility property of the drug candidate.

7. The method of claim 1 wherein the biosensor utilizes a mass-sensing technique.

8. The method of claim 7 wherein the mass-sensing technique involves surface plasmon resonance.

9. The method of claim 1 wherein the at least one mathematical expression correlated from binding interaction data associated with known drug compounds is a function fitted to a plurality of data points plotted on a Cartesian coordinate system.

10. The method of claim 1 wherein the plurality of sensing surface-bound biomolecules are selected from liposomes, plasma proteins, CYP 450 enzymes, metabolic enzymes, or transport proteins.

11. The method of claim 1 wherein the biosensor utilizes a sensor chip comprising:

a hydrogel coupled to the sensor surface, wherein the hydrogel has a plurality of functional groups, and wherein the one or more sensing surface-bound biomolecules are bonded to the hydrogel.

12. The method of claim 11 wherein the sensor chip further comprises:

a free electron metal that includes a sensor surface, wherein the free electron metal is selected from the group consisting of copper, silver, aluminum and gold.

13. The method of claim 12 wherein the biosensor is capable of detecting surface plasmon resonance associated with the free electron metal.

14. The method of claim 12 wherein the hydrogel is a polysaccharide or a water-swellable organic polymer.

15. The method of claim 14 wherein the polysaccharide is dextran.

16. The method of claim 11 wherein the plurality of functional groups of the hydrogel of the sensor chip include one or more of a hydroxyl, carboxyl, amino, aldehyde, carbonyl, epoxy or vinyl functional group.

17. The method of claim 11 wherein the step of measuring comprises detecting a signal associated with a reflected light beam with respect to time, wherein the reflected light beam establishes a surface plasmon resonance with the free electron metal.

18. The method of claim 17 wherein the signal associated with the reflected light beam defines a resonance curve of the surface plasmon resonance.

19. The method of claim 17 wherein the signal associated with the reflected light beam defines a reflectance minimum of the surface plasmon resonance.

20. A computer memory containing a data structure useful for assaying a drug candidate in accordance with the method of claim 1, the data structure comprising binding interaction data associated with known drug compounds such that the data structure may be used to determine an estimate of at least one pharmacokinetic parameter of the drug candidate.

21. A generated data signal for conveying a data structure useful for assaying a drug candidate in accordance with claim 1, the data structure comprising binding

interaction data associated with known drug compounds such that the data structure may be used to determine an estimate of at least one pharmacokinetic parameter of the drug candidate.

22. An apparatus for assaying a drug candidate, the apparatus comprising a biosensor having one or more sensing surface-bound biomolecules associated therewith and capable of measuring at least one binding interaction parameter of the drug candidate, and a computer memory containing a data structure for comparing the at least one binding interaction parameter against at least one mathematical expression correlated from binding interaction data associated with known drug compounds to determine an estimate of at least one pharmacokinetic parameter of the drug candidate.

23. The apparatus of claim 22 wherein the at least one pharmacokinetic parameter is an absorption parameter, a distribution parameter, a metabolism parameter, or an excretion parameter.

24. The apparatus of claim 22 wherein the at least one pharmacokinetic parameter is volume of distribution, total clearance, protein binding, tissue binding, metabolic clearance, renal clearance, hepatic clearance, biliary clearance, intestinal absorption, bioavailability, relative bioavailability, intrinsic clearance, mean residence time, maximum rate of metabolism, Michaelis-Menten constant, partitioning coefficients between tissues and blood or plasma, fraction excreted unchanged in urine, fraction of drug systemically converted to metabolites, elimination rate constant, half-life, or secretion clearance.

25. The apparatus of claim 24 wherein the partitioning coefficients between tissues and blood or plasma are partitioning coefficients associated with the blood brain barrier, blood placenta barrier, blood human milk partitioning, blood adipose tissue partitioning, or blood muscle partitioning.

26. The apparatus of claim 22 wherein an estimate of at least two pharmacokinetic parameters of the drug candidate are determined.

27. The apparatus of claim 22 wherein the biosensor utilizes a mass-sensing technique.

28. The apparatus of claim 27 wherein the mass-sensing technique involves surface plasmon resonance.

29. The apparatus of claim 28 wherein the at least one mathematical expression correlated from binding interaction data associated with known drug compounds is a function fitted to a plurality of data points plotted on a Cartesian coordinate system.

30. The apparatus of claim 22 wherein the plurality of sensing surface-bound biomolecules are selected from liposomes, plasma proteins, CYP 450 enzymes, metabolic enzymes, or transport proteins.

31. The apparatus of claim 22 wherein the biosensor utilizes a sensor chip comprising:

a hydrogel coupled to the sensor surface, wherein the hydrogel has a plurality of functional groups, and wherein the one or more sensing surface-bound biomolecules are bonded to the hydrogel.

32. The apparatus of claim 31 wherein the sensor chip further comprises:

a free electron metal that includes a sensor surface, wherein the free electron metal is selected from the group consisting of copper, silver, aluminum and gold.

33. The apparatus of claim 32 wherein the biosensor is capable of detecting surface plasmon resonance associated with the free electron metal.

34. The apparatus of claim 32 wherein the hydrogel is a polysaccharide or a water-swellable organic polymer.

35. The apparatus claim 34 wherein the polysaccharide is dextran.

36. The apparatus of claim 31 wherein the plurality of functional groups of the hydrogel of the sensor chip include one or more of a hydroxyl, carboxyl, amino, aldehyde, carbonyl, epoxy or vinyl functional group.

37. The apparatus of claim 31 wherein a signal associated with a reflected light beam with respect to time is detected, and wherein the reflected light beam establishes a surface plasmon resonance with the free electron metal.

38. The apparatus of claim 37 wherein the signal associated with the reflected light beam defines a resonance curve of the surface plasmon resonance.

39. The apparatus of claim 37 wherein the signal associated with the reflected light beam defines a reflectance minimum of the surface plasmon resonance.

40. A sensor surface adapted for use with a biosensor, comprising:

a hydrogel matrix coating coupled to a top surface of the sensor surface, wherein the hydrogel matrix coating has a plurality of functional groups; and

at least two different types of liposomes bonded to the plurality of functional groups, wherein the at least two different types of liposomes are at discrete and noncontiguous locations on the hydrogel matrix coating of the sensor surface.

41. The sensor surface of claim 40 wherein a free electron metal is interposed between the hydrogel matrix and the top surface of the sensor surface, wherein the free electron metal is selected from the group consisting of copper, silver, aluminum and gold.

42. The sensor surface of claim 40, further comprising at least one lipophilic substance interposed between the at least two different types of liposomes and the plurality of functional groups, wherein the lipophilic substance is covalently bonded to the plurality of functional groups.

43. The sensor surface of claim 42 wherein the lipophilic substance comprises an alkyl chain having from 12 to 24 carbon atoms.

44. The sensor surface of claim 42 wherein the lipophilic substance is stearylamine.

45. The sensor surface of claim 40 wherein the at least two different liposomes are 1,2-dimyristol-*sn*-glycero-3-phosphocholine (DMPC) and 1-palmitoyl-2-oleoyl-*sn*-glycero-3-phosphocholine (POPC).

46. The sensor surface of claim 40, further comprising human serum albumin bonded to the plurality of functional groups at discrete and noncontiguous locations on the hydrogel matrix coating of the sensor surface.

47. The sensor surface of claim 40, further comprising one or more of a CYP 450 enzyme, a metabolic enzyme, or transport protein bonded to the plurality of functional groups at discrete and noncontiguous locations on the hydrogel matrix coating of the sensor surface.